Supplementary Information

Probing the microscopic structure and flexibility of oxidized DNA by molecular simulations

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S.1 Persistence length using $P(\theta) \sim e^{-\frac{\beta\kappa}{2L_0}(\theta-\theta_0)^2}$

Considering the intrinsic curvature of dsDNA duplex, we subtracted the angle $\theta_0 = \langle\theta\rangle$ of the equilibrated structure in each bending angle θ and used it to compute the persistence length.

With this approach, the equations 1 and 2 of the main article take following forms.

$$P(\theta) = \sqrt{\frac{\beta\kappa}{2\pi L_0}} e^{-\frac{\beta\kappa}{2L_0}(\theta-\theta_0)^2} \tag{S.1}$$

where, θ_0 is the time average of the bending angle of the duplex over all frames. With it, $\theta' = \theta - \theta_0$ is the bending angle of the duplex with respect to its equilibrated structure.

For small angle $\theta' = \theta - \theta_0$, equation S.1 can be approximated as:

$$lnP(\theta) = -\frac{l_p}{L_0}(1 - cos\theta') + \frac{1}{2}ln\Big(\frac{\beta\kappa}{2\pi L_0}\Big) \tag{S.2}$$

where, $\kappa = \frac{l_p}{\beta} = K_B T l_p$ is the bending modulus, T is temperature of the system in Kelvin, and K_B is the Boltzmann's constant. From the slope of the graph of $lnP(\theta)$ versus $(1 - cos\theta')$ we can compute the persistence length using: $slope = -\frac{l_p}{L_0}$.

With it, the new values of persistence lengths are slightly changed from the results presented in the main article but follow the same trend. The results with this approach and the approach used in the main article are presented in the table St.1.

Table St.1: Persistence lengths using equation 1 (of main article) and equation S.1

System	Persistence Length(l_p) in nm **[a]**	Persistence Length(l_p) in nm **[b]**
	Using $P(\theta) \sim e^{-\frac{l_p}{2L_0}\theta^2}$	Using $P(\theta) \sim e^{-\frac{l_p}{2L_0}(\theta-\theta_0)^2}$
dsDNA	48.87 ± 1.81	53.13 ± 2.93
dsDNA(4oxG)	58.61 ± 2.06	62.87 ± 4.02
dsDNA(80xG)	61.31 ± 2.44	67.28 ± 3.25

The procedures followed in computing the persistence lengths l_p are based on the theories of Mazur[1] and Mogurampelly et al.[2] Here, **[a]** corresponds to the approach used in the main article and **[b]** corresponds to the approach used in this supplementary information (SI). Using the two approaches, the l_p values are found to vary slightly but follow the same trend described in the main article.

Linear fit plots for contour length and bending angle data of the duplexes:

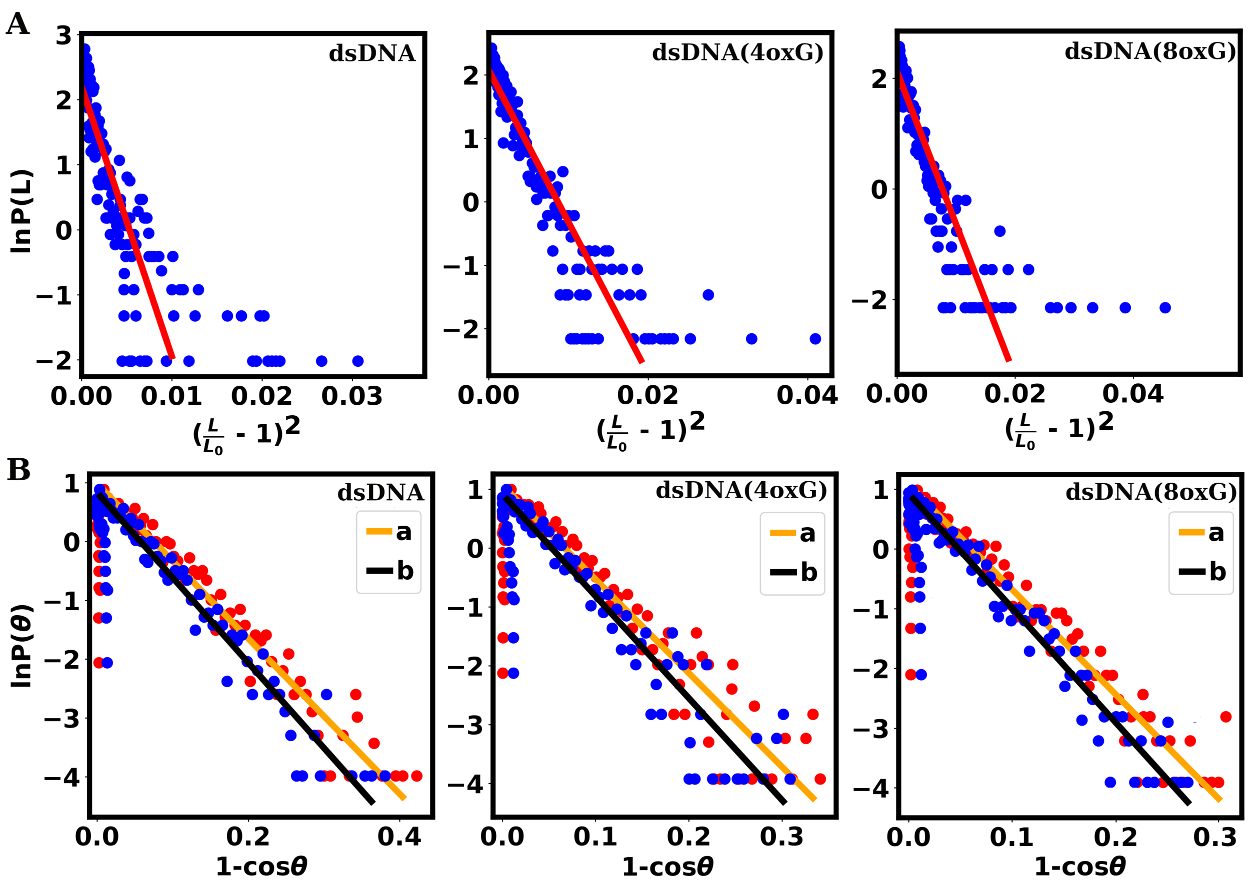

Figure SF. 1: Linear fit plots. **[A]**: $lnP(L)$ versus $(\frac{L}{L_0}-1)^2$ and **[B]**: $lnP(\theta)$ versus $(1-cos\theta)$. In lower panel, **a** corresponds to the line obtained with equation $lnP(\theta) = -\frac{l_p}{L_0}(1-cos\theta) + \frac{1}{2}ln\left(\frac{\beta\kappa}{2\pi L_0}\right)$ and **b** corresponds to the line obtained with equation $lnP(\theta) = -\frac{l_p}{L_0}(1-cos\theta') + \frac{1}{2}ln\left(\frac{\beta\kappa}{2\pi L_0}\right)$.

S.2 Backbone torsion angles of the duplexes

Table St.2: Averages of backbone torsion angles and sugar puckers

Torsion	Duplex	**2_I**	**4_I**	**7_I**	**10_I**	**14_II**	**16_II**	**19_II**	**22_II**
α	dsDNA	282.52 (18.44)	287.49 (12.15)	293.85 (11.03)	286.47 (14.72)	283.89 (15.54)	287.26 (12.22)	293.84 (9.93)	282.82 (30.02)
	dsDNA(4oxG)	278.08 (45.11)	286.21 (11.51)	294.52 (9.88)	285.86 (19.40)	284.86 (26.85)	285.51 16.80	294.56 (10.12)	284.91 (13.15)
	dsDNA(8oxG)	264.49 (61.33)	280.20 (25.27)	294.71 (9.95)	282.59 (28.82)	274.68 41.19	282.83 (12.88)	294.42 (13.54)	280.84 (34.21)
β	dsDNA	162.42 (23.94)	161.09 (18.35)	180.26 (16.60)	162.66 (21.16)	161.01 (23.19)	160.88 (18.38)	179.36 (16.46)	163.09 (21.6)
	dsDNA(4oxG)	168.14 (16.13)	165.19 (11.44)	177.90 (16.36)	161.90 (20.16)	167.74 (16.26)	165.38 (12.01)	178.96 (16.54)	162.30 (19.99)
	dsDNA(8oxG)	172.92 (19.29)	166.62 (12.17)	176.26 (16.10)	169.11 (11.91)	172.12 (18.19)	166.49 (11.37)	176.41 (16.43)	169.11 (12.10)
γ	dsDNA	52.48 (19.05)	52.44 (11.05)	55.48 (8.68)	51.40 (14.29)	51.01 (13.86)	52.14 (11.40)	55.37 (8.69)	53.44 (23.29)
	dsDNA(4oxG)	58.92 (38.68)	51.31 (9.06)	56.18 (8.69)	50.71 (20.2)	53.63 (19.31)	51.76 (12.38)	56.17 (8.77)	49.75 (14.12)
	dsDNA(8oxG)	71.73 (37.22)	51.25 (19.44)	56.47 (8.82)	50.97 (28.17)	56.86 (42.18)	49.21 (10.40)	56.66 (11.86)	52.75 (34.01)
ε	dsDNA	192.93 (33.83)	221.65 (42.13)	180.40 (14.33)	204.85 (40.56)	192.61 (32.29)	222.18 (41.58)	180.34 (14.56)	204.15 (39.36)
	dsDNA(4oxG)	258.89 (23.04)	256.05 (22.05)	179.34 (14.21)	207.64 (40.41)	259.48 (22.58)	256.01 (21.98)	179.41 (13.87)	208.96 (41.51)
	dsDNA(8oxG)	261.61 (23.54)	257.60 (21.77)	179.32 (13.42)	262.66 (20.37)	260.77 (23.31)	257.49 (21.84)	179.13 (13.58)	261.99 (20.83)
ζ	dsDNA	251.59 (40.18)	214.49 (50.53)	266.53 (13.91)	236.30 (50.08)	252.27 (14.60)	214.61 (50.61)	266.46 (14.24)	237.71 49.27
	dsDNA(4oxG)	162.16 (20.29)	169.14 (18.16)	267.31 (13.24)	235.44 (51.19)	161.75 (20.49)	169.18 (17.98)	267.35 (12.98)	233.10 (52.18)
	dsDNA(8oxG)	160.35 (22.76)	166.85 (18.42)	267.42 (12.87)	159.25 (18.87)	161.49 (21.50)	167.10 (18.31)	267.52 (12.73)	159.56 (18.85)
ε - ζ	dsDNA	-58.65 (72.14)	7.15 (91.04)	-86.12 (25.29)	-31.45 (89.08)	-59.97 (68.98)	7.56 (90.52)	-86.10 (25.91)	-33.56 (86.89)
	dsDNA(4oxG)	96.72 (40.57)	86.91 (37.21)	-87.96 (24.47)	-27.80 (90.14)	97.73 (40.71)	86.83 (36.77)	-87.94 (23.75)	-24.14 (92.18)
	dsDNA(8oxG)	101.26 (43.79)	90.74 (37.18)	-88.10 (23.25)	103.41 37.12	99.29 42.26	90.39 37.12	-88.39 23.22	102.43 37.31
χ	dsDNA	253.75 (14.97)	259.60 (15.19)	244.61 (13.12)	254.36 (14.56)	252.27 (14.60)	259.75 (15.19)	244.27 (13.29)	253.45 (15.11)
	dsDNA(4oxG)	263.53 (13.93)	268.59 (12.68)	241.88 (13.64)	254.65 (14.67)	264.62 (14.50)	262.97 (12.48)	241.81 (13.61)	254.90 (14.43)
	dsDNA(8oxG)	264.01 (15.18)	267.32 (12.85)	240.78 (13.73)	264.39 (12.78)	263.60 (15.24)	263.68 (12.79)	240.86 (13.73)	264.62 (12.86)
ϕ	dsDNA	165.54 (24.01)	152.97 (23.63)	138.13 (24.05)	160.69 (25.90)	164.99 (24.83)	153.38 (23.96)	137.11 24.99	160.97 27.22
	dsDNA(4oxG)	140.47 (17.80)	142.02 (13.68)	134.71 (24.51)	160.84 (24.40)	139.69 (16.41)	141.96 (14.08)	137.32 (24.49)	160.52 (23.94)
	dsDNA(8oxG)	142.27 (20.87)	139.37 (13.17)	132.47 (24.67)	139.19 (14.34)	139.43 (17.70)	139.27 (12.59)	136.84 (24.56)	139.56 (15.21)
ν_m	dsDNA	36.60 (7.14)	40.48 (7.34)	37.63 (6.33)	38.10 (7.57)	36.67 (7.01)	40.44 (7.42)	37.65 (6.33)	37.96 (7.72)
	dsDNA(4oxG)	45.21 (5.89)	44.58 (5.14)	38.05 (6.38)	38.57 (7.85)	45.01 (5.95)	44.56 (5.23)	38.08 (6.33)	38.81 (7.89)
	dsDNA(8oxG)	45.24 (6.34)	46.10 (5.01)	38.38 (6.37)	46.88 (5.28)	45.87 (6.05)	46.10 (5.04)	38.26 (6.35)	46.65 (5.43)

Mean and standard deviation (shown in parentheses) of backbone torsion angles, sugar ring pucker amplitude (ν_m), and phase angle (ϕ). All values are in degree.

References

(1) Mazur, A. K. Wormlike Chain Theory and Bending of Short DNA. *Phys. Rev. Lett.* **2007**, *98*, 218102.

(2) Mogurampelly, S.; Nandy, B.; Netz, R. R.; Maiti, P. K. Elasticity of DNA and the effect of dendrimer binding. *The European Physical Journal E* **2013**, *36*, 68.